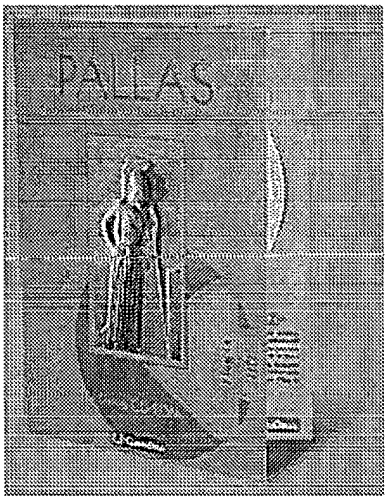
You can find on our homepage all the latest information on our software & directly access the pages of our software products.

Windows Products:

Pallas Classic:

Including programs for pK_a log*P*, log*D* predictions, Metabolism & Toxicity , HPLC dev lopment: pKalc , PrologP , PrologD , MetabolExpert , HazardExpert , Eluex



Pallas Plug-in:

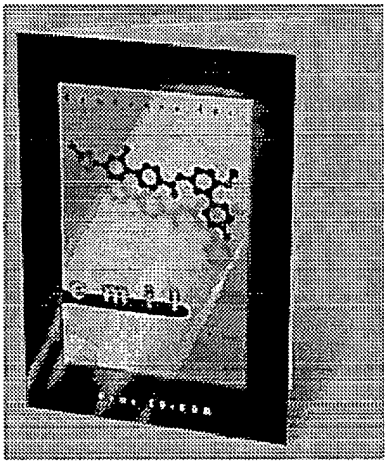
Contains add-in modules for use in the ISIS/BASE system: Pallas Plug-in for ISIS™*

Unix (Irix, Solaris, Linux) DLL:

Implement the three determinative modules into your system. pKalc, PrologP, PrologD can be bought as a DLL or as Unix version.

Lead Evolution: EMIL (Example-Mediated Innovation for Lead-Evolution)

In collaboration with 16 leading Japanese pharmaceutical companies ComGenex has developed a new software EMIL.
This is an advisory system for chemical development which includes many structural evolution examples from a wide range of the literature examples as well as a structural generation engine to give structural examples. Please visit this page to explore how EMIL can you extend the functionality of your own structure database.



CompuDrug Support

Update & latest news

- Pallas systems are Windows 2000 compliant.
- Upgraded pKalc: the pKalc 5.0 version. If you have valid maintenance agreement

with CompuDrug and want to download the latest update, please click here. The download is possible only with your personal password and key only. To receive your password and key, please contact us with your registration number and details.

- If you are a user of Pallas 2.0 and have not yet received your updated version of Pallas, please contact us.

Other support within the site

- If you would like additional copies of Users Guides please download here.
- If you have any question about our products, please contact us by e-mail.
- Click here to download free demo versions of our latest products.
- Overseas visitors please go to our European mirror site.
- The site-map will help you to navigate around our site.

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Take a visit at our mother company's site:



pKalc 5.0 for Windows

The world's first commercial program for calculating pK_a from the structure of the compound

Theo. Background

PKa is the negative logarithm of the ionisation constant (Ka), which is related to the acidity and basicity of a compounds.

Assuming that substituents cause free energy changes, which can be added linearly, pKalc uses Hammett and Taft equations to perform each calculation. These equations describe the dissociation equilibrium of organic acids and bases, together with s substituent constants.

pKalc is especially helpful for calculating pK_a values when the experimental determination of pK_a values is difficult, or impossible. This situation occurs when the substance has a low water solubility or when the substance is unstable in water. It can provide assistance with weak acids and bases, with unstable materials and with insufficiently soluble substances.

To download the pKalc manual click here

Features

- Predicts pK_a values in aqueous phase
- Indicates acidic and basic pK_a values
- Uses large KB (more than 600 ionizable centres and 800 substituents)
- Lowest acidic and highest basic pK_a values are considered
- Effect of ionized substituents are taken into account
- Exporting results to any spreadsheet editor (in TAB delimited text file format)

2K1 other updates: inclusion of a database of an experimental pK_a values

Implemented an experimental database the pKalc program has been updated with additional option. Using more than 12,000 measured compound the program has a large database including approximately 60,000 experimental pK_a values which will allow the user to get additional results and information on the measured compound. The database is one of the largest collections of experimental pK_a values. The database search happens during displaying the results and the experimental values can be found at the end of the results, but there is no significant change in the usage of the software.

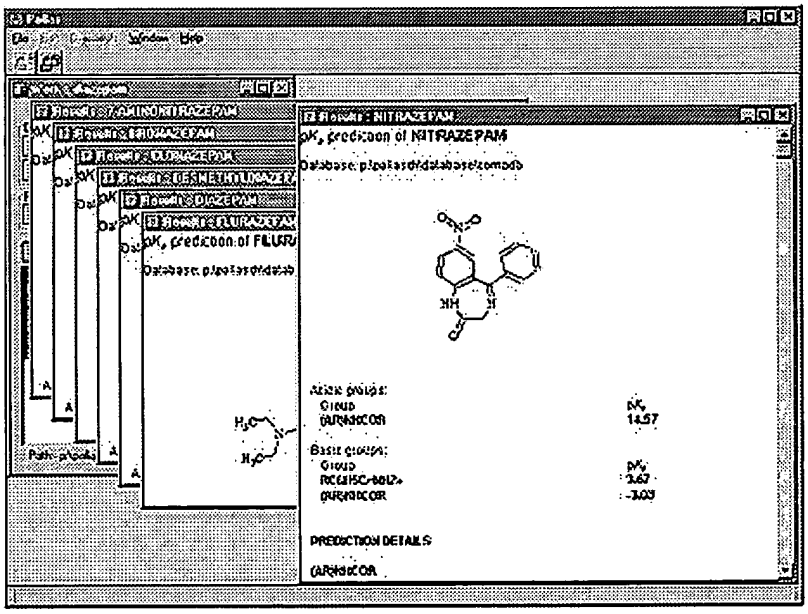
pKalc 5.0 upgrade

PKaWizard has been implemented into Pallas pKalc program to help the user in preparation of new Hammett/Taft equations. It drives the user through the definition of the ionizable centers and the corresponding equation step by step, taking care of the possible mistakes and giving a hand in problematic situations. For definition of ionizable centers a graphical interface is implemented into pKaWizard, which is responsible for the proper settings of the positive and negative structural conditions. At the final step of the equation building procedure a regression plot is given and the user can check out the parameters of the new Hammet/Taft equation.

Areas of Use

- Analytical
- Medicinal
- Drug design
- Absorption
- Preparative
- Separative
- For defining the pH of the mobile phase
- pKalc is espécially helpful when the experimental determination of pK_a is difficult or impossible. This situation occurs when the substance has a low water solubility or when the substance is unstable in water.

Snapshot



Hw. Requirements

- IBM compatible 486 computer, min. 8 MB RAM
- All Windows operating system
- One floppy disk drive
- One hard disk drive with 5 MB free space

- Mouse or trackball
- Optional printer

DLL version is also available

Main Page

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